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14. ABSTRACT

We examine the problem of uniqueness in the relationship between the remote-sensing reflectance (Rrs) and the inherent optical properties (lOPs) of ocean water. The results point to the fact that diffuse reflectance of plane irradiance from ocean water is inherently ambiguous. Furthermore, in the 400 < X < 750 nm region of the spectrum, Rrs(X) also suffers from ambiguity caused by the similarity in wavelength dependence of the coefficients of absorption by particulate matter and of absorption by-colored dissolved organic matter. The absorption coefficients have overlapping exponential responses, which lead to the fact that more than one combination of lOPs can produce nearly the same Rrs spectrum. This ambiguity in absorption parameters demands that we identify the regions of the Ers spectrum where we can isolate the effects that are due only to scattering by particulates and to absorption by pure water. The results indicate that the spectral shape of the absorption coefficient of phytoplankton, aPh(X), cannot be derived from a multiparameter fit to Rrs(X). However, the magnitude and the spectral dependence of the absorption coefficient can be estimated from the difference between the measured Rrs(X) and the best fit to Rrs(X) in terms of lOPs that exclude aPh(X).

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Uniqueness in remote sensing of the inherent optical properties of ocean water

Michael Sydor, Richard W. Gould, Robert A. Arnone, Vladimir I. Haltrin, and Wesley Goode

We examine the problem of uniqueness in the relationship between the remote-sensing reflectance (Rrs) and the inherent optical properties (IOPs) of ocean water. The results point to the fact that diffuse reflectance of plane irradiance from ocean water is inherently ambiguous. Furthermore, in the $400 < \lambda < 750$ nm region of the spectrum, Rrs(λ) also suffers from ambiguity caused by the similarity in wavelength dependence of the coefficients of absorption by particulate matter and of absorption by colored dissolved organic matter. The absorption coefficients have overlapping exponential responses, which lead to the fact that more than one combination of IOPs can produce nearly the same Rrs spectrum. This ambiguity in absorption parameters demands that we identify the regions of the Rrs spectrum where we can isolate the effects that are due only to scattering by particulates and to absorption by pure water. The results indicate that the spectral shape of the absorption coefficient of phytoplankton, $a_{\mathrm{ph}}(\lambda)$, cannot be derived from a multiparameter fit to Rrs(λ). However, the magnitude and the spectral dependence of the absorption coefficient can be estimated from the difference between the measured Rrs(λ) and the best fit to Rrs(λ) in terms of IOPs that exclude $a_{\mathrm{ph}}(\lambda)$. © 2004 Optical Society of America

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1. Introduction

This investigation was prompted by two questions raised at the recent Ocean Optics XVI Conference in Santa Fe, New Mexico, on 18–23 November 2002:

1. Why do we have trouble with remote-sensing algorithms for the inherent optical properties (IOPs) of ocean water in certain areas of the oceans where colored dissolved organic matter (CDOM) is present; i.e., why are algorithms for IOPs not global?
2. Why do we need hyperspectral measurements of remote sensing reflectance [Rrs(λ)] rather than measure Rrs at few well-placed wavelengths to retrieve IOPs by use of remote-sensing data?

These questions lead us to examine the uniqueness of the spectral shapes of Rrs(λ) as a function of wavelength λ. Mobley[1] raised the question of uniqueness some decade ago. Uniqueness implies that we cannot have two different sets of parameters that predict the same reflectance spectrum within the experimental accuracy. To test uniqueness or to prove the ambiguity of Rrs(λ) we need to examine its mathematical definition and devise two or more distinct sets of parameters or two mathematical solutions that yield equivalent Rrs spectra.

To avoid possible preselection of data in testing for ambiguity of Rrs(λ) we examine data published by other investigators as well as our own recent data from experiments from the Gulf of Mexico. In particular, we make impromptu use of data presented by Roesler and Boss[2] at the scientific conference mentioned above. The examination of Rrs from widely disparate sources and geographic regions will lend global character to our investigation and will leads us to a better understanding of the underlying physical processes that give rise to Rrs.

Let us first examine the accepted mathematical expressions for diffuse reflectance R from ocean water in terms of IOPs. Gordon *et al.*[3] give R as

$$R = f b_b/(a + b_b), \tag{1}$$

where b_b is the volume backscattering coefficient and a is the total volume absorption coefficient, which is composed of the sum of $a_y(\lambda)$, $a_d(\lambda)$, $a_w(\lambda)$, and $a_{\mathrm{ph}}(\lambda)$, the absorption by CDOM, detritus, pure water, and phytoplankton, respectively; see Ref. 1. Factor f is a

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constant of proportionality whose magnitude depends on the definition of reflectance. For reflectance of plane irradiance f is ~0.33 and R is defined as E_u/E_d^-, the ratio of upwelling irradiance E_u to downwelling irradiance E_d^-, where both quantities in this ratio are measured just beneath the water surface. Equation (1) provides the accepted wavelength dependence for variety of other expressions for reflectance from ocean water. Thus the in-water reflectance Rrsw, defined as L_u/E_d^- by Jerome *et al.*,[4] is also given in terms of the wavelength dependence of $b_b/(a + b_b)$ according to

$$\text{Rrsw} = (f/Q)b_b/(a + b_b), \tag{2}$$

where L_u is the upwelling radiance and $Q = E_u/L_u$ is a factor given by Morel and Prieur[5] that accounts for the bidirectionality of the Rrsw. In a detailed investigation of the properties of Q, Morel *et al.*[6] show that Q varies with wavelength in a complex manner. This fact would limit the usefulness of Eq. (2). However, it appears that the quotient $f/Q \sim 0.1$ remains nearly constant, independently of wavelength and solar angle, for protocol observation of the Rrsw.[1]

The most commonly used expression for the reflectance from ocean water is Rrs. It is the all-important reflectance in optical monitoring of oceans by satellites. It is defined as L_w/E_d, the ratio of water-leaving radiance L_w and irradiance E_d just above the water surface. By accounting for the transmittance of light at the air–water and water–air interfaces, denoted tt', and taking into account the spread in the solid angle as L_u emerges from water to become L_w, we obtain

$$\text{Rrs} = \{(f/Q)(tt'/n_R^2)\}b_b/(a + b_b) \quad [\text{sr}^{-1}], \tag{3}$$

where n_R is the relative index of refraction for the air–water interface [for Eq. (3) we assume flat surface conditions, and the equation is not exact; see Ref. 1]. Again, the coefficient in braces in Eq. (3) is deemed nearly independent of λ.

By referencing all the above expressions for reflectance to plane irradiance E_d we in essence disregard the angular distribution of the incident light. However, scattering from marine particles is highly directional; therefore reflectance from ocean water is also a directional quantity whose magnitude and spectral shape depend on the angular distribution of the incident light. Thus referencing Rrs(λ) to E_d makes Rrs(λ) inherently ambiguous because in principle we can obtain the same $E_d(\lambda)$ for more than one intensity of incident light. For instance, two different angular distributions of daylight illuminating the same water mass can give the same E_d but different Rrs and vice versa. One could argue that such differences are negligible in practice for good protocol observational conditions that specify the observational angles for Rrs relative to the Sun. Perhaps this is true, but we shall see that there is another, more tangible, difficulty when it comes to the question of uniqueness of Rrs(λ).

Inasmuch as the combination of factors in front of the term $b_b/(a + b_b)$ in Eqs. (1)–(3) is usually treated as a constant of proportionality, we tacitly imply that the wavelength dependence of Rrs(λ) comes from the wavelength dependence of $b_b/(a + b_b)$. Ladner *et al.*[7] used *in situ* measurements of $b_b(\lambda)$ together with measurements of $a(\lambda)$ to show that $b_b/(a + b_b)$ does not correlate with Rrs(λ) in the visible region of the spectrum. Some of the discrepancy presented by Ladner *et al.*[7] may come from the lack of accuracy in measurements of $b_b(\lambda)$. Determination of $b_b(\lambda)$ is vulnerable to error when $b_b(\lambda)$ is measured at one or a few angles that avoid the anomalous backscattering at 180°; see Ref. 8.

Sydor[9] provides an alternative solution for Rrs(λ) that is not based on $b_b(\lambda)$. Using statistical consideration of multiple scattering, Sydor[9] gives Rrs at any λ in terms of the average number of scatters per photon, b/a. The full relationship between Rrs and b/a is given by

$$\text{Rrs}/(1 - 2\pi\text{Rrs}) \sim C_b b/a, \tag{4}$$

where C_b has the value 0.001 ± 0.0002 for waters that obey Petzold[10] volume scattering function for coastal waters. The term $(1 - 2\pi\text{Rrs})$ in relation (4) comes from the correction for the number of scatters per photon in a semi-infinite medium. For an infinite medium the number of scatters per photon is $n = (b/a)$. The number of scatters per photon in a semi-infinite medium reduces to $(b/a)(1 - 2\pi\text{Rrs})$ because of reflectance. Photons can escape the semi-infinite medium before they scatter an average of n times. For $\text{Rrs} \ll 1/(2\pi)$ the left-hand side of relation (4) becomes Rrs, and relation (4) simplifies to $\text{Rrs} \approx C_b(b/a)$.[11] Relation (4) provides an alternative solution to Eq. (3) because it gives Rrs in terms of the dimensionless angle-independent ratio b/a that is easier to verify experimentally. Measurement of $a(\lambda)$ and $b(\lambda)$ is routine in ocean optics. Relation (4) differs fundamentally from Eq. (3) because, in the former, $b(\lambda)$ and $b_b(\lambda)$ need not have the same wavelength dependence. By using the dependence of Rrs on b/a, Sydor *et al.*[11] showed that taking $\text{Rrs} \approx C_b(b/a)$ provides good estimates of IOPs from Rrs, provided that Rrs is analyzed in a sequential manner that starts with the determination of $b(\lambda)$ from the spectral region where a_w dominates the absorption. Sydor *et al.*[11] used experimental data for the waters of Lake Superior and the Mississippi Sound to show that the proportionality between Rrsw and b/a is compatible with the polynomial expression for Rrsw presented by Jerome *et al.*[4] In general, relation (4) states that Rrs is not a linear function of IOPs.

The differences in solutions such as Eq. (3) and relation (4) are paramount in discussion of uniqueness. Even if we assume that b_b/b is nearly independent of wavelength, Eq. (3) and relation (4) differ mathematically. Thus, if both solutions provide nearly the same Rrs(λ), then Rrs(λ) cannot be truly unique. Sydor *et al.*[11] have already shown that more than one set of $b(\lambda)$ and $a(\lambda)$ can produce similar Rrs(λ) in the visible region of the spectrum, where

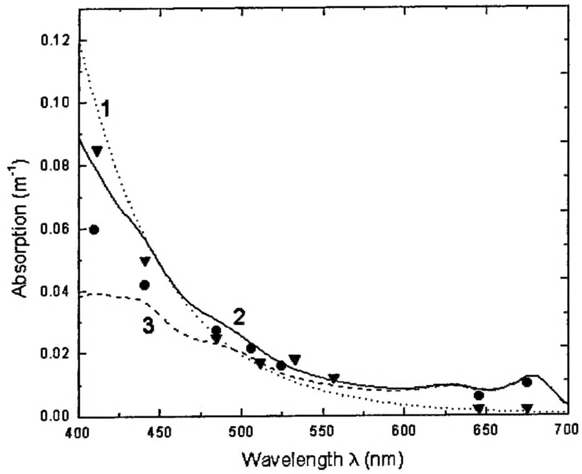

Fig. 1. Spectral absorption coefficients derived from relation (4) applied in sequential fit to Rrs(λ) off the coast of South Africa before the onset of phytoplankton bloom. 1, 2, 3, Predicted a_y, a_p, a_{ph}, respectively. Rrs(λ) was traced from enlarged figures shown by Roesler and Boss.[2] Solid and filled triangles and circles, a_y and a_p, respectively, taken from Roesler and Boss. The wavelength dependence of the surrogate $a_{ph}{}^*(\lambda)$ used in the sequential fit was based on $a_{ph}(\lambda)$ measured in the waters of the Mississippi Sound (Ref. 11). The magnitude of $a_{ph}(\lambda)$ shown here corresponds roughly to $0.038a_{ph}{}^*(\lambda)$. No attempt was made to back out the actual $a_{ph}(\lambda)$ spectrum off the coast of South Africa. We assumed that $a_w(\lambda)$ dominated $a(\lambda)$ for $\lambda > 650$ nm. This assumption is justified because at 650 nm $a_{w650} \sim 0.35\ \mathrm{m}^{-1}$, which is far greater than the combined values of a_d, a_{ph}, and a_y at 650 nm reported by Roesler and Boss.

Rrs(λ) depends on some nine variable parameters. We test their result further by fitting Rrs(λ) with measured IOPs, using both Eq. (3) and relation (4).

2. Experimental Results

By using neural networks, Roesler and Boss[2] employed a version of Eq. (1) modified in terms of extinction coefficient $c(\lambda)$ to extract IOPs from Rrs(λ) and R(λ). They made the assumption that b_b/b is a weak function of λ and minimized the ambiguity in Rrs(λ) by procedural methods in their neural networks technique. The use of neural networks in analysis of Rrs(λ) is novel, but in fact it is still a least-squares fit. We performed a similar task on the data of Roesler and Boss[2] but employed a least-squares fit to Rrs(λ), using relation (4) and employing a sequential parameter fit that starts with the determination of $b(\lambda)$ in the spectral region where $a(\lambda)$ is dominated by $a_w(\lambda)$.

First we considered the Rrs data of Roesler and Boss[2] taken off the coast of South Africa. Using a simplified form of relation (4) we estimated the magnitude of b_{730} from the slope of Rrs(λ) versus $[C_b/(\lambda a_w)]$ for $\lambda > 650$ (nm), where we took $C_b = 0.0011\ \mathrm{sr}^{-1}$ and assumed that $b(\lambda)$ behaves as $\sim(1/\lambda)$. The result yielded $b(\lambda) \sim 0.4(730/\lambda)\ m^{-1}$. Subsequently we determined the components of $a(\lambda)$ by following the procedure described by Sydor *et al.*[11] The results of this procedure are in close agreement with the experimental data for Rrs(λ), as shown in Fig. 1.

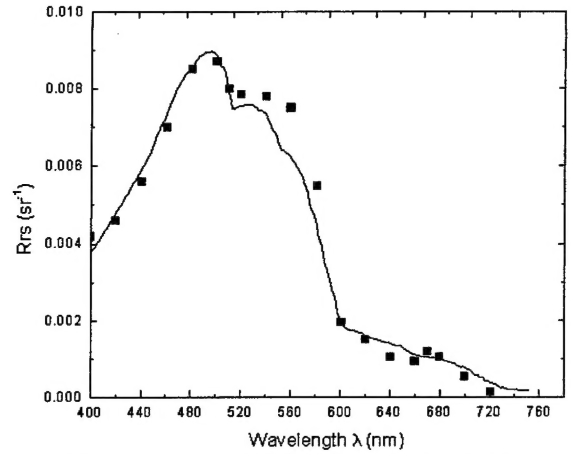

Fig. 2. Filled squares, Rrs(λ) off the coast of South Africa taken from Ref. 2. Solid curve, sequential fit to Rrs(λ) based on relation (4) with $C_b = 0.0011$ and $b(\lambda) = 0.39(730/\lambda)^{1.1}$.

The resultant fit to the Rrs of Roesler and Boss[2] is shown in Fig. 2. The correlation for the fit in Fig. 2 gave $r^2 = 0.99$, as demonstrated in Fig. 3. Thus we obtained a result equivalent to that of Roesler and Boss[2] by using a different fitting routine, different IOP parameters, different assumptions, and different equations, confirming that the relationship between Rrs and IOPs is ambiguous.

To examine the root cause of this ambiguity further, we used the data of Roesler and Boss[2] for $R(\lambda)$ taken off the coast of Oregon. The use of $R(\lambda)$ rather than Rrs(λ) is important because $R(\lambda)$ is presumably devoid of the inaccuracies that are due to atmospheric and surface corrections. By using the sequential least-squares fit to $R(\lambda)$ we again estimated $b(\lambda)$ from a plot of $R(\lambda)$ versus $(C_b'/\lambda a_w)$, assuming in this case that $a_w(\lambda)$ dominates $a(\lambda)$ for $\lambda > 560$ nm. For reflectance R, $C_b' \sim \pi(n_R{}^2/tt')C_b \sim 0.0065$. The procedure yielded $b(\lambda) \sim 0.1(730/\lambda)\ \mathrm{m}^{-1}$. This magnitude of $b(\lambda)$ indicates that the scattering in the waters off the Oregon Coast is dominated by suspended particles. Molecular scattering is 60 times

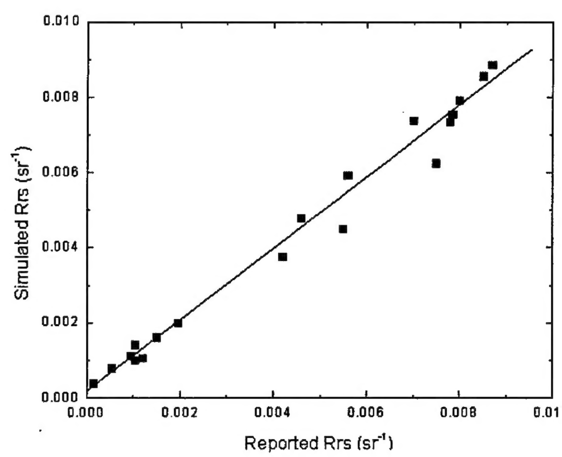

Fig. 3. Solid line, $r^2 = 0.99$ correlation between sequentially simulated Rrs(λ) and reported Rrs(λ) (filled squares from Fig. 2).

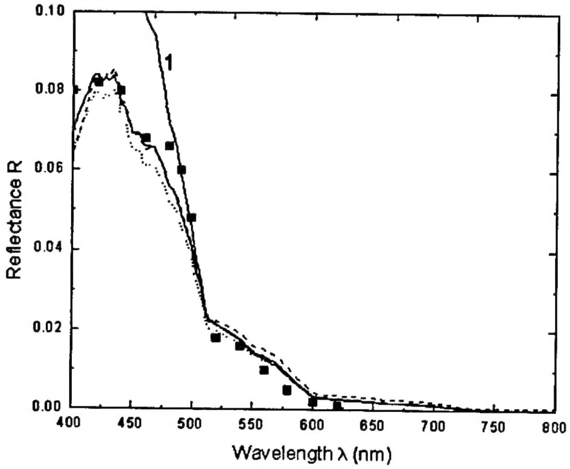

Fig. 4. Filled squares, reflectance $R(\lambda)$ off the coast of Oregon. The data were traced from Roesler and Boss.[2] Close fits to this $R(\lambda)$ can be obtained by use of real and false sets of IOP parameters. Dotted curve, first-order sequential fit without any iteration. Solid curve, sequential parameter fit by iteration to find the best fit. Dashed curve, example of an *ad hoc* parameter fit. The contrived *ad hoc* fit departs from the experimental $R(\lambda)$ at longer wavelengths where a_w dominates the absorption and thereby limits the possibility of a false fit. Curve 1, fit from use of $0.0065b/a_w$ alone, indicating that in this case $1/(\lambda a_w)$ determines the spectral shape of $R(\lambda)$ for $\lambda > 500$ nm.

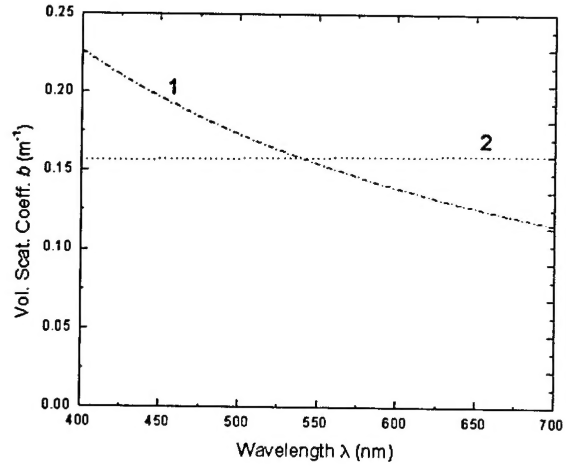

Fig. 5. Curve 1, $b(\lambda)$ determined from $R(\lambda)$ versus C_b'/a_w in the $\lambda > 560$ nm region of $R(\lambda)$ shown by the filled squares in Fig. 4. Curve 2, $b(\lambda)$ for the false *ad hoc* fit to $R(\lambda)$. $b(\lambda)$ obtained in the *ad hoc* fit is deemed unlikely, as its magnitude increases with λ. Nonetheless, the *ad hoc* $b(\lambda)$ produces a close fit to $R(\lambda)$ as long as $a_d(\lambda)$ and $a_y(\lambda)$ are adjusted accordingly.

lower[1] than our $b(\lambda) \sim 0.1(730/\lambda)\ \mathrm{m}^{-1}$. As a result, in applying the sequential fit to $R(\lambda)$ we ignored molecular scattering. On the other hand, Roesler and Boss[2] included molecular scattering in their neural fitting routine for $R(\lambda)$; thus they increased the number of variable parameters even further than that used in our least-squares sequential fit. Figure 4 shows the least-squares fit to $R(\lambda)$ off the Oregon Coast. The correlation for $R(\lambda)$ was $r^2 \sim 0.99$, comparable with the result of Roesler and Boss[2] but without the use of the extra parameters that are due to molecular scattering.

The results in Fig. 4 demonstrate the ambiguity of reflectance from ocean water in the visible region of the spectrum and simply point to the fact that any broad function of λ such as $\mathrm{Rrs}(\lambda)$ or $R(\lambda)$ can be approximated closely by more than one combination of broad functions such as $b(\lambda)$, $a_y(\lambda)$, and $a_d(\lambda)$ that together have several adjustable parameters; the greater the number of parameters, the greater the ambiguity. To demonstrate this ambiguity caused by overparameterization of $R(\lambda)$ we produced an *ad hoc* fit to $R(\lambda)$ by neglecting $a_{\mathrm{ph}}(\lambda)$ altogether and varying at will the magnitude and the wavelength dependence of $b(\lambda)$ and $a(\lambda)$ without a_{ph} until we came up with a close fit to the experimental $R(\lambda)$. The *ad hoc* fit is also shown in Fig. 4. We can see that it approximates the measured $R(\lambda)$ with $r^2 \sim 0.98$ or better. The scattering and the absorption coefficients for the sequential and the *ad hoc* fits are shown in Figs. 5 and 6, respectively. The *ad hoc* $b(\lambda)$ in Fig. 5 is deemed unlikely because its magnitude increases with the wavelength, whereas $b(\lambda)$ usually decreases as $\sim(1/\lambda)$. Yet the unlikely $b(\lambda)$ provides an excellent fit to $R(\lambda)$ for $\lambda < 500$ nm as long as we adjust $a(\lambda)$ accordingly. Basically, any unrestricted fit to $\mathrm{Rrs}(\lambda)$ would lead to a similar result, because any given $\mathrm{Rrs}(\lambda)$ does not translate to a unique combination of IOPs in ocean water; see Ref. 1. Clearly the situation is not hopeless because we can restrict

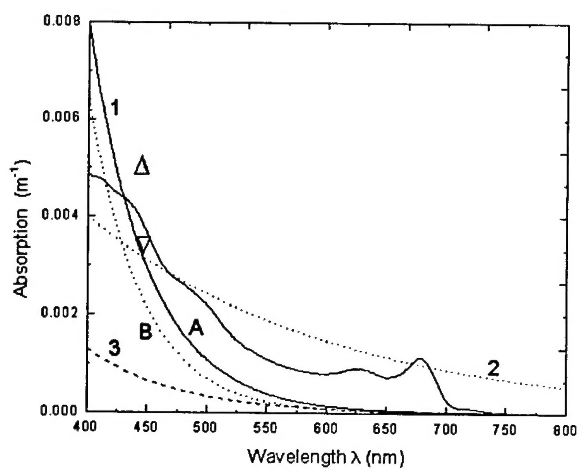

Fig. 6. The solid trace and curve 2 show $a_p(\lambda)$ from the sequential and the *ad hoc* fits, respectively, to $R(\lambda)$ off the Oregon Coast (filled squares in Fig. 4). Curve 3, $a_d(\lambda)$, the detrital component of $a_p(\lambda)$. Most of the absorption by suspended particles off the Coast of Oregon is attributable to $a_{\mathrm{ph}}(\lambda)$, whose magnitude here was $0.0035a_{\mathrm{ph}}{}^*(\lambda)$ of the waters of the Mississippi Sound. The lone upward-pointing triangle shows an experimental point for a_p reported by Roesler and Boss.[2] Curves A and B, $a_y(\lambda)$ for the sequential and the *ad hoc* fits, respectively. The downward-pointing triangle shows the lone a_y point reported by Roesler and Boss.[2] We assumed that a_w dominates the absorption in the tail of $R(\lambda)$ for $\lambda > 560$ nm. Curve 1 of Fig. 4 shows that this assumption was justified. The pure-water tail, where $a_w(\lambda) \sim a(\lambda)$, shifts toward the shorter wavelengths when the concentration of suspended particles and CDOM is low.

and prioritize the search for reasonable IOPs by knowing the general properties of IOPs for any area ahead of the time. Nonetheless, the fact that any given Rrs(λ) does not represent a unique set of IOPs places a limit on the accuracy of the remote-sensing determination of IOPs, especially $a_{\mathrm{ph}}(\lambda)$, whose *a priori* wavelength dependence is always uncertain.

The upshot of the above presentation is that we need some prior knowledge of the wavelength dependence of IOPs when we try to determine IOPs remotely. For instance, any fitting routine that takes advantage of the fact that $1/[\lambda a_w(\lambda)]$ determines the spectral shape of Rrs(λ) in a long-wavelength tail is likely to select a realistic value for $b(\lambda)$ and subsequently determine a realistic $a(\lambda)$ relative to the known magnitude of $a_w(\lambda)$.[11] Consider, for example, $R(\lambda)$ of off the Coast of Oregon. Half of its spectral shape, the region $\lambda > 500$ nm, is determined solely by $1/(\lambda a_w)$, as demonstrated by curve 1 in Fig. 4. In general, we can provide reasonable approximations to Rrs(λ) or $R(\lambda)$ based on the expected exponential dependence of $a_y(\lambda)$ and $a_d(\lambda)$ and the $\sim 1/\lambda$ dependence of $b(\lambda)$. Subsequently we can back out $a_{\mathrm{ph}}(\lambda)$ that provides a perfect fit to Rrs(λ) as shown in Ref. 11. However, we can never be sure of the accuracy of $a_{\mathrm{ph}}(\lambda)$ because we are never sure of the surface corrections for Rrs(λ) and the inherent ambiguity in Rrs that is due to the uncertainty in the angular distribution of the incident light.

Much of the ambiguity that is attributable to overparameterization comes from the fact that a_y and a_d have similar overlapping exponential dependence on λ.[11] Thus the relative contributions from a_y and a_d to the total $a(\lambda)$ can produce a variety of close approximations to any given Rrs spectrum. Clearly, no matter what fitting routines we use, the ambiguity produced by the similarity of the wavelength dependence of $a_y(\lambda)$ and $a_d(\lambda)$ could never be resolved if $a_y(\lambda)$ and $a_d(\lambda)$ had exactly the same wavelength dependence. The overparameterization vanishes in the tail of Rrs(λ) because a_y and a_d drop off exponentially while a_w increases rapidly as $\lambda \rightarrow 700$ nm. For $\lambda > 750$ nm, all absorption coefficients become negligible except for a_w; thus we can use this region of the spectrum to isolate the dependence of Rrs(λ) on $b(\lambda)$.

To examine the discrepancy in Rrs(λ) represented by Eq. (3) versus Rrs expressed in terms of b/a, we examined Rrs for Pearl River, Miss., and the Gulf of Mexico. Figure 7 shows Rrs(λ) for the turbid waters of the Pearl River. It also shows the least-squares fit from relation (4) and the expected Rrs(λ) using *in situ* measurements of $b_b(\lambda)$, $b(\lambda)$, $a_y(\lambda)$, $a_d(\lambda)$, and $a_{\mathrm{ph}}(\lambda)$ in Eq. (3) and relation (4). All magnitudes of Rrs in Fig. 7 were normalized to the measured Rrs at 620 nm to permit comparison of the wavelength dependence predicted by each equation. The measured and simulated IOPs of Pearl River waters are shown in Figs. 8 and 9. If we take $b_b(\lambda)$ measured by use of a Hydroscat instrument at face value, the result shown in Fig. 7 demonstrates that Eq. (3) does not produce a close fit to Rrs(λ). The shortcoming of Eq. (3) applied to measuring the highly turbid Pearl

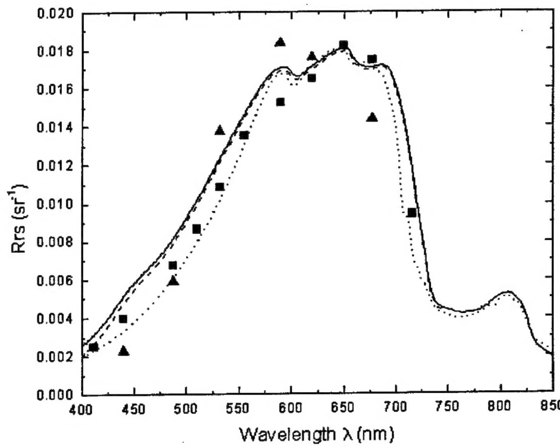

Fig. 7. Wavelength dependence of Rrs(λ) for turbid waters of Pearl River, Miss. Solid and dashed curves, two (independently) surface corrected values of Rrs(λ) for Pearl River. The triangles show that $b_b/(a + b_b)$ does not follow the measured Rrs(λ); the filled squares show that $(b/a)(1 - 2\pi\mathrm{Rrs})$ follows the spectral shape of Rrs(λ) quite closely. To compare their spectral dependence we normalized both cases to the measured Rrs at 620 nm. The dotted curve shows that the sequential fit to Rrs(λ) has the correct magnitude and displays the fine spectral features exhibited in the measured Rrs(λ).

River is not surprising. Whitlock *et al.*[12] suggested that Eq. (3) fails for turbid waters. Ladner *et al.*[7] demonstrated a similar result in their Fig. 5. In fact, their data show[7] that Rrs does not correlate well with $b_b/(a + b_b)$ for $\lambda < 650$ nm but that the correlation improves markedly for $\lambda > 676$ nm, where the wavelength dependence of $b_b(\lambda)$ and $b(\lambda)$ becomes similar, as indicated in Fig. 8. The similarity of the wavelength dependence of $b(\lambda)$ and $b_b(\lambda)$ for $\lambda > 676$ nm could be attributed to the fact that a_p may affect b_b (owing to the electromagnetic boundary conditions on the illuminated side of the particles) more than it

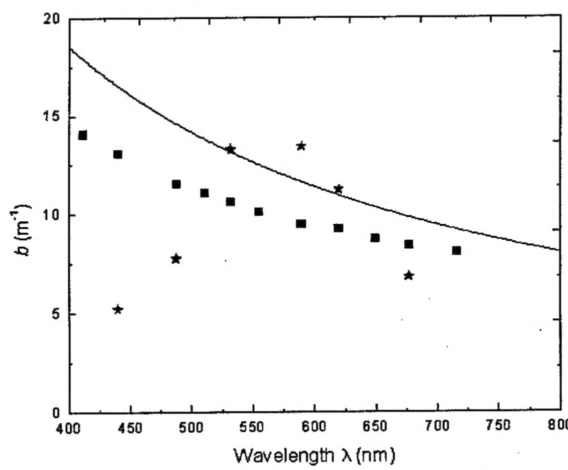

Fig. 8. Filled squares, $b(\lambda)$ for Pearl River determined with an ac9 instrument. Stars, $b_b(\lambda)$ measured with Hydroscat (multiplied here by a factor of 14 to permit its wavelength dependence to be compared with that of $b(\lambda)$). Solid curve, $b(\lambda)$ obtained from a sequential fit by use of relation (4) and $C_b = 0.0012$ sr^{-1}.

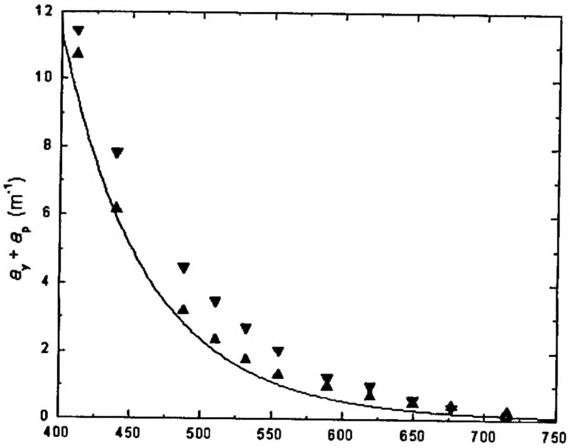

Fig. 9. Downward-pointing triangles $a(\lambda)$ (without a_w) for the waters of Pearl River, Miss. Upward-pointing triangles, the sum of $a_y(\lambda)$ measured with a 0.045-μm pore filter at the intake of the ac9 meter plus $a_p(\lambda)$ determined from a filter-pad transmission measurement. Solid curve, $a(\lambda)$ obtained from the sequential fit from relation (4).

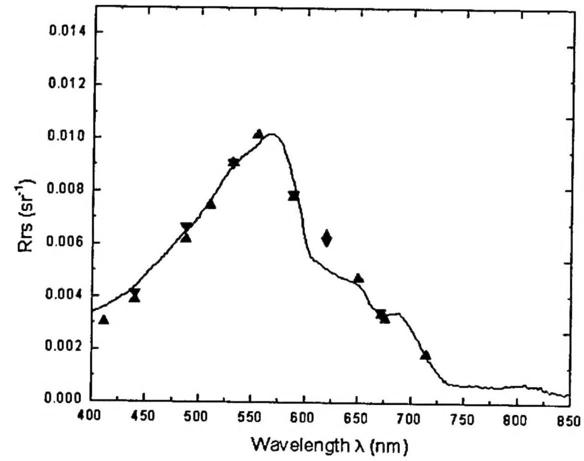

Fig. 10. In the linear limit of Rrs $\ll 1$ and constant $b_b/b < 0.03$, Eq. (3) and relation (4) give comparable results for Rrs(λ). Downward-pointing triangles, Rrs(λ) obtained from Eq. (3) by Hydroscat $b_b(\lambda)$ and ac9 measurement of $a(\lambda)$. Upward-pointing triangles, Rrs(λ) predicted by relation (4) from ac9-determined $b(\lambda)$ and $a(\lambda)$. Solid curve, measured Rrs(λ).

affects the total b. Thus, when $a_p(\lambda) \rightarrow 0$ as $\lambda \rightarrow 700$ nm, b_b and b attain a similar wavelength dependence that depends only on the particle size distribution and on the average index of refraction; then the correlation between Rrs and $b_b/(a + b_b)$ improves.

By comparing the values of Rrs predicted by Eq. (3) and relation (4) we can see from Fig. 7 that relation (4) produces a closer fit to the measured Rrs(λ) because it accounts for all scattering. What can we conclude from such results? The underlying laws of physics are not ambiguous and should produce only one correct result. If diffuse reflectance were referenced to the incident radiance rather than irradiance, Rrs would be defined uniquely, but the problem of overspecification would remain. Terms such as f/Q are designed to account for the distribution of the incident radiance and multiple scattering. However, f/Q introduces its own ambiguity because additional variables tend to disguise the inadequacy of Eq. (3) that arises from the fact that Rrs cannot be described solely in terms of the plane-wave single backscattering process that is implied by use of b_b in Eq. (3). For extended illumination and multiple scattering, forward scattering also contributes to the spectral dependence of Rrs(λ). Indeed, photons observed in Rrs come from variety of combinations of forward and backward scattering whose combined average wavelength dependence governs the wavelength dependence of Rrs(λ). In multiple scattering each reflected photon samples a variety of particles in a process that is fundamentally different from that represented by b_b, where by definition each photon samples one particle only. Thus in multiple scattering the sampling of the optical properties of suspended particles is interrelated from one scatter to the next. As a result, Rrs from multiple scattering is not additive, as implied by single-scattering equation (3) for which each photon scatters only once and samples the optical properties one particle at a time independently of other particles. Rrs from multiple scattering is not a linear function of IOPs. Relation (4) includes multiple scattering and photon turnaround through computation of the magnitude of C_b.[9] It states that average Rrs(λ) is proportional to $(b/a)(1 - 2\pi\text{Rrs})$, the average number of scatters per photon in a semi-infinite medium. Thus relation (4) states that Rrs $= 0$ only if $b = 0$. Equation (3) does not account for photon turnaround and states that Rrs $\rightarrow 0$ if $b_b \rightarrow 0$ even if b is finite. This is clearly erroneous. Equation (3) and relation (4) approach the same result in the linear limit of Rrs $\ll 1$ and constant $b_b/b < 0.03$, as demonstrated experimentally by Rrs(λ) in Fig. 10. In the linear limit, binomial expansion of Eq. (3) and relation (4) shows that they differ largely in the magnitude of the proportionality constant.

3. Need for Hyperspectral Data

We can resolve the ambiguity from overparameterization by identifying the region of the spectrum where a_w dominates the absorption. However, the pure-water region shifts toward the shorter wavelengths, depending on the concentration of suspended particles and CDOM. To monitor a wide variety of ocean waters one needs Rrs(λ) data that cover the entire 380–950-nm spectrum with a sufficient number of bands that the location of the shifting spectral region where $a_w(\lambda) \sim a(\lambda)$ can be identified. The upper wavelength limit at 950 nm is needed as the point of reference where Rrs becomes negligible because $a_w \rightarrow 30$ m^{-1}; i.e., where we can set the magnitude of the atmospherically corrected Rrs at zero and use it to estimate the magnitude of the rough-surface reflectance.[11] Similarly, Shybanov[13] points out that the region near 380 nm is useful for estimating the magnitude of a_y.

4. Conclusions

Rrs(λ) does not correspond to a unique set of IOPs. Values of IOP close to those of the actual IOPs can be obtained from spectral analysis of Rrs(λ), provided that we impose realistic limits on the wavelength dependence of $b(\lambda)$, $a_y(\lambda)$, and $a_d(\lambda)$. Usually $b(\lambda)$ has a smooth monotonic $\sim 1/\lambda$ dependence, unlike $b_b(\lambda)$. Thus, by using relation (4) under the condition that $\mathrm{Rrs} \ll 1$ and $a \sim a_w$, we can estimate the magnitude of $b(\lambda)$ from plots of Rrs(λ) versus $C_b/(\lambda a_w)$. C_b varies by 20% with particle concentration but appears constant as a function of λ, and its average magnitude, 0.001 sr^{-1}, appears to hold for a variety of coastal waters. However, it is unlikely that C_b is global outside the limits $0.01 < b_b/b < 0.04$ set by Jerome *et al.*[4] It is also unlikely that Eq. (3) is global for open ocean waters where CDOM is present.

We have made use of data presented by Roesler and Boss[2] and by Ladner *et al.*[7] published in the proceedings of the Ocean Optics XVI Conference in Santa Fe, N.Mex. on 18–23 November 2002. We are indebted to those investigators for sharing their results. We are also grateful to our colleague Al Weidermann for personal communications and for providing us with data on the spectral dependence of the scattering phase function measured by Misha E. Lee and Eugene B. Shybanov.

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